UNDERSTANDING THE SIZE EFFECT IN THE MECHANICAL PROPERTIES OF NANOTWINNED COPPER

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Summary We performed large-scale molecular dynamics simulations to study the plastic deformation of nanotwinned polycrystalline copper. Our simulations showed that the materials' plastic deformation was initiated by partial dislocation nucleations at grain boundary triple junctions. Although both dislocation cutting across twin boundaries and dislocation-induced twin migrations were observed, our quantitative analysis revealed that the cutting interaction through a Lomer dislocation mechanism was the dominant one. We further examined the effect of twin spacing on this dominant mechanism through a series of specifically-designed nanotwinned copper samples over a wide range of twin spacing. The simulations showed that a transition in the dominant deformation mechanism occurred at a small critical twin spacing. Based on these observations, a simple, analytical model for the critical twin spacing was proposed and the predicted critical twin spacing was shown to be in excellent agreement both with respect to the atomistic simulations and experimental observation.

INTRODUCTION

Changing microstructural length scales has often been used to manipulate the mechanical properties of metals. Recently, manipulation of microstructural characters has drawn considerable attention. Twins are found especially good for controlling strength because of their extraordinary stability [1]. Remarkably, some nanotwinned metals paradoxically exhibit both high strength and high ductility. Lu *et al*. [2] demonstrated that in pure, nanotwinned Cu, the yield strength exhibits a maximum strength at a small, finite twin spacing. In addition, they found that while the strength goes through a maximum at a critical twin spacing, the strain hardening and ductility increase monotonically with decreasing twin spacing. Earlier simulations [3,4] were unable to reproduce this transition in strengthening behavior at twin spacings below the experimentally observed critical twin spacing at about 15 nm. Interestingly, a recent molecular dynamics (MD) study [5] demonstrated a softening mechanism arising from the nucleation from the cutting of a twin boundary with a grain boundary and gliding of dislocations parallel to twin boundaries at small twin spacings (0.63 to 1.25 nm). They suggested the plastic deformation in this unique microstructure switched from strengthening based on dislocation pile-ups to softening through twin migrations. It is noticed, however, that high resolution TEM observations [2] of those after-deformation nanotwinned Cu samples showed a high density of dislocations blocked at twin boundaries for samples having a small twin spacing (4 nm). The genesis of these dislocations is not clear in the current literature. Comparison of the after-deformation MD results with TEM images indicates that, apart from the reported mechanism switch [5], there might be other mechanisms operative when the twin spacing was changed. In addition, the existence of a maximum in the strength, with no minimum in the ductility and strain hardening, suggests the existence of an unrecognized length scale in the strength of this unusual metal. In this paper, we performed large-scale MD simulations of polycrystalline Cu with nanotwins. Our simulation results suggest an additional deformation mechanism change when the twin spacing is below a critical value.

SIMULATION MODEL AND METHOD

Molecular dynamics simulations were performed using the Lammps Molecular Dynamics Simulator [7] in which the atomic trajectories were determined by integrating the equations of motion for each atom in the system. The interactions between copper atoms were described using the Embedded Atom Method (EAM) [8] potential parametrized by Mishin [9]. This potential was fitted to experimental and ab initio data of copper and was shown to accurately reproduce many material properties, including the stacking fault energy -- an important property in deformation studies. In the MD simulations, periodic boundary conditions were imposed in all directions. The temperature and the stress tensor were adjusted through a Nose/Hoover temperature thermostat and pressure barostat, respectively.

SIMULATION RESUTLS AND DISCUSSION

Our MD simulations showed that the onset of plastic deformation started when leading partial dislocations were first nucleated at grain boundary triple junctions. These newly nucleated partial dislocations glided and created wide stacking faults (10 nm) until they were blocked by twin boundaries. Both pure screw and 60^{o} dislocations started to

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cross twin boundaries. Those screw dislocations crossed twin boundaries by slipping on {111} and $\{111\}^T$ planes in the matrix and twin grains alternatively. This process kept the twin boundary intact. The interactions of 60^o dislocations with twin boundaries were different from those pure screw ones. Lomer dislocations were frequently formed on the $\{001\}^T$ plane in the next twin crystal when the dislocations passed through a twin boundary. It was found that such Lomer dislocations were able to cross-slip and dissociate into Shockley and stair-rod dislocations, provided that the dislocation line segments were pure screw. In addition to the dislocation twin boundary interactions, twin migrations through partial dislocation gliding on twinning boundaries were also observed in some grains, which was attributed as the softening mechanism in a recent study [5]. However, our quantitative analysis showed that the twin migration mechanism was less dominant when the twin spacing was above 2 nm.

We further performed an extensive study on the deformation mechanism of nanotwinned Cu as a function of twin spacing. We identified a change in deformation mechanism at a small twin spacing and showed that this change in mechanism occurred at a twin spacing that was consistent with the experimentally-observed critical one for softening. At large twin spacing (18.8 nm), Lomer dislocations were formed. As the Lomer dislocation line evolved, part of the dislocation line rotated such that its line direction became parallel to its Burgers vector; thus forming a pure Lomer screw dislocation. This pure screw segment was observed to cross-slip and dissociate into Shockley partial dislocations a stair-rod dislocation. Through the cross-slip and dissociation of Lomer dislocations, the system develops a complicated 3D dislocation structure containing both glissile and sessile dislocations on various slip planes. Examining the deformation process in simulations performed at small twin spacings, we found that the process of cross-slip and dissociation of Lomer dislocations did not occur. Instead, slip was constrained to the original slip system such that a two dimensional dislocation microstructure was formed.

As discussed above, our polycrystalline simulation demonstrated frequent occurrences of the Lomer dislocation formation and dissociation mechanism. Since Lomer dislocations were formed frequently in our simulation and their dissociation mechanism depended on the radius of curvature, we used these results to develop a model for the twin spacing at which the classical increase in strength with decreasing microstructural length scale broke down and provided a simple approach to predicting the critical twin spacing for the mechanism transition. This critical twin spacing is in consistent with the experimental observation.

Earlier studies [2] suggested the plastic deformation process in this unique microstructure was related to dislocation-twin interactions. Dislocation tangles and networks were observed in samples with large twin spacings while planar dislocations associated with twin boundaries (and twin steps) were formed in samples with small twin spacings. The two different dislocation mechanisms operating at large and small twin spacings first reported here resulted in dislocation pattern which is consistent with the above experimental facts. Hence the mechanism suggested in this paper matches closely not only in the transition length scale but also in the resultant dislocation pattern.

CONCLUSIONS

We presented large-scale MD simulation on plastic deformation of polycrystalline nanotwinned Cu. It was found that dislocation nucleations from grain boundary triple junctions initiated plastic deformation in the simulation. Both pure screw and 60^o dislocations crossing over twin boundaries were observed in our simulation and the later generated Lomer dislocations which further dissociated into various Shockley and stair-rod partial dislocations. We further performed simulations over a wide range of twin spacing and revealed a transition in the deformation mechanism at a small, critical twin spacing. Based upon these observations, we proposed an analytical model for the critical twin spacing scale. Comparison of the predicted critical twin spacing with both our MD results and experimental data showed that the model led to an excellent agreement, confirming our assertion that the transition of dislocation mechanism is a source for the experimentally observed transition of the strength in nanotwinned copper with twin spacing.

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